

ENERGY HIGH PERFORMANCE COMPUTING CONFERENCE



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FEBRUARY 25-27, 2025
HOUSTON, TEXAS



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Responsible AI and Computing for Global Impact

The Ken Kennedy Institute at Rice University is pleased to host the 18th annual Energy High Performance Computing Conference in Houston, TX. The Energy HPC Conference is the premier meeting place for key stakeholders to engage in conversations about challenges, opportunities, and developments impacting the energy industry. The program includes invited speakers, technical talks, and birds of a feather sessions that combine diverse insights and perspectives from industry, academia, and national labs, as well as an exhibit hall, networking receptions, poster presentations, and add-on workshops.

The Ken Kennedy Institute at Rice University is committed to addressing critical global challenges through foundational research in AI and computing. Our collaborative, interdisciplinary approach drives discoveries and responsible innovation across scientific disciplines. In pursuit of that mission, we hope that this event serves as a meeting place for researchers, engineers, and industry professionals to build connections and engage with local and global HPC and AI communities.

We are grateful to our sponsors, ecosystem partners, speakers, and attendees who share our enthusiasm for this annual gathering. A special thank you is due for our sponsors, as proceeds from this conference contribute to recruiting fellowships for prospective graduate students to attend Rice University as well as industry-sponsored fellowships to propel current graduate students in their education and provide connections with professionals in the field. These efforts enable us to support the next generation of researchers in computational science and engineering, AI, and machine learning. Since 2012, the Energy HPC Conference has funded 88 fellowships totaling over \$650,000.

The Ken Kennedy Institute team would also like to recognize Keith Gray, conference co-founder and VP for Computational Science and Engineering at TotalEnergies, along with our phenomenal conference committee for their many contributions to this year's program — this highly-anticipated event exists because of your efforts.

On behalf of the conference committee, Rice University, and the Ken Kennedy Institute, we thank you for being here.

Lydia E. Kavraki, PhD

Director, Ken Kennedy Institute

David V. Pynadath, PhD

Executive Director for Research Initiatives, Ken Kennedy Institute

CONFERENCE COMMITTEE

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The Ken Kennedy Institute, established in 1986, is an interdisciplinary group committed to addressing critical global challenges through foundational research in AI and Computing. The Institute fosters collaborative efforts to drive AI-powered discoveries across diverse scientific disciplines and champions ethical and responsible AI innovation.

We cannot achieve our mission without meaningful connections and valuable insight. Please contact us with your questions and ideas at kenkenney@rice.edu.



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Conference Code of Conduct

The organizers invite all attendees, sponsors/exhibitors, speakers, media, volunteers, and other participants to help us realize a safe and positive conference experience for everyone. The Ken Kennedy Institute works to increase tolerance, opportunity, and diversity in an effort to continually encourage the open exchange of ideas. For these reasons,

the Institute is committed to providing a harassment-free experience at all the events it organizes. If you experience or witness harassment or discriminatory behavior at the conference, report this promptly to kenkenney@rice.edu.

The conference venue is shared with members of the public that are not

attendees of the conference; please be respectful to all patrons of these locations.

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2025

ENERGY HIGH PERFORMANCE COMPUTING CONFERENCE

INVITED CONFERENCE SPEAKERS



Prasanna Balaprakash
*Oak Ridge National
Laboratory*



Biondo Biondi
Stanford University



Jesse Chan
Rice University



Melyssa Fratkin
*Texas Advanced
Computing Center (TACC)*



Selda Günsel
Shell Technology



Daniel (Dan) Reed
University of Utah



Dan Stanzione
*Texas Advanced Computing
Center (TACC); The University
of Texas at Austin*



Timothy Williams
*Argonne National
Laboratory*

2024-2025 Ken Kennedy Institute Sponsored Fellowship Recipients



Rice Ken Kennedy Institute Graduate Fellowship Award Recipients (*top row, from left to right*): Yu-Neng (Allen) Chuang, Anindita Dash, Hossein Gazmeh, Dragana Grbic, Catherine He, Arnold Kazadi, Ziran Wang, Yihua Xu, Nicolas Zilberstein



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Excellence in Computer Science**



**Scott Morton Memorial
Graduate Fellowship**

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The Ken Kennedy Institute is pleased to recognize the achievements and research of Rice University's graduate students by awarding fellowships to students pursuing research related to high performance computing, computational science and engineering, and data science. Fellowship awards are made possible with support from our Corporate Partners bp, ExxonMobil and Shell, the Energy High Performance Computing Conference, and the Andrew Ladd, Ken Kennedy-HPE Cray, and Scott Morton endowments.

We aim to continue expanding our fellowship opportunities beyond the energy sector to include disciplines in healthcare and public health for upcoming award cycles. To learn more about sponsoring a graduate fellowship, please email kenkenedy@rice.edu.



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Ken Kennedy Institute Computational Science & Engineering Graduate Recruiting Fellowships

Funded by the proceeds from the Ken Kennedy Institute's Energy High Performance Computing Conference, the goal of this fellowship program is to attract exceptional graduate students to Rice University the fields of high performance computing, computational science and engineering, and data science, with special consideration given to students with research interests in areas of relevance to the energy industry.

2024-2028 Recipients

Saisrinivas (Sri) Gudivada

Applied Physics

Aleksandr Gulkanov

Mechanical Engineering

Nikki Hart

Computer Science

Daniel Illera

Statistics

Yangqianzi (Qianzi) Jiang

Statistics

Lingxi Zhang

Computer Science

Siyuan Tao

Bioengineering

Xiaobei (Emma) Zhang

Applied Physics

2023-2027

Alexander Ahrens

Applied Physics

Cesar Cardenas

Statistics

Khushbu Pahwa

Computer Science

Xiaorong Zhang

Electrical & Computer Engineering

2022-2026

Brianna Barrow

Computer Science

Alyssa Cantu

Computer Science

Rose Graves

Statistics

Kevin McCoy

Statistics

John Steinman

Computational Applied Mathematics & Operations Research

Ria Stevens

Computer Science

Xiaoyu (Rosie) Zhu

Earth, Environmental, and Planetary Sciences

2021-2025

Kelsey Murphy

Earth, Environmental, and Planetary Sciences

Jose Palacio

Statistics

Xinyu (Xin) Yao

Computer Science

2025 PROGRAM | TUESDAY, FEBRUARY 25

W Add-On Workshop

B Birds of a Feather (BOF)

M Main Session

N Networking

A Technical Talk: Domain Science and AI

R Technical Talk: HPC for Research

S Technical Talk: Innovation and Sustainability

E Technical Talk: Programming and Systems Efficiency

8:00 a.m. – 8:30 a.m.

N Check-in + Breakfast **>>** Auditorium + Exhibit Hall

8:30 a.m. – 9:30 a.m.

B BOF I Sustainability: Energy Effectiveness and Cooling Future Processors and Accelerators **>>** Auditorium

Speaker(s): **Peter de Bock**, Advanced Research Projects Agency-Energy (ARPA-E); **Keith Gray**, TotalEnergies; **Michael Gujral**, Shell; **Greg Huff**, Lenovo; **Tommy Minyard**, Texas Advanced Computing Center (TACC); **Tejas Shah**, Intel Corporation; **Austin Shelnutt**, Strategic Thermal Labs; **Punith Shivaprasad**, Shell; **Mark Steinke**, NVIDIA

9:30 a.m. – 10:00 a.m.

N Morning Coffee Break **>>** Exhibit Hall

10:00 a.m. – 10:10 a.m.

M Welcome I Day 1 **>>** Auditorium

Speaker(s): **Amy Dittmar**, Rice University; **Lydia Kavraki**, Ken Kennedy Institute, Rice University; **Keith Gray**, TotalEnergies

10:10 a.m. – 10:55 a.m.

M Keynote I HPC and Applied Seismology: A Long and Successful Partnership **>>** Auditorium

Speaker(s): **Biondo Biondi**, Stanford University

10:55 a.m. – 11:30 a.m.

M AI and HPC, or AI Ends HPC? **>>** Auditorium

Speaker(s): **Dan Stanzione**, Texas Advanced Computing Center (TACC); The University of Texas at Austin

11:30 a.m. – 12:20 p.m.

N Lunch **>>** Exhibit Hall

12:20 p.m. – 2:05 p.m.

S Technical Talks: Innovation and Sustainability **>>** Auditorium

12:20 p.m. – 2:05 p.m.

R Technical Talks: HPC for Research **>>** Second Floor, Room 280

2:05 p.m. – 2:40 p.m.

N Afternoon Break **>>** Exhibit Hall

2:40 p.m. – 3:15 p.m.

M Overview of Oak Ridge National Laboratory's AI Initiative: Advancing Secure, Trustworthy, and Energy-Efficient AI at Scale for Scientific Discovery **>>** Auditorium

Speaker(s): **Prasanna Balaprakash**, Oak Ridge National Laboratory (ORNL)

3:15 p.m. – 3:50 p.m.

M Efficient Implementation of High Order Entropy Stable Methods for Computational Fluid Dynamics **>>** Auditorium

Speaker(s): **Jesse Chan**, Rice University

3:50 p.m. – 5:30 p.m.

N Sponsor Networking Reception **>>** Exhibit Hall

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Technical Talks: Innovation and Sustainability >> Auditorium

- | | |
|--------------------------------|--|
| 12:20 p.m. – 12:55 p.m. | Five Big Questions for HPC-AI in 2025
Speaker(s): Addison Snell, Intersect360 Research |
| 12:55 p.m. – 1:30 p.m. | Bridging Academia and Industry: Enhancing Wind Resource and Yield Energy Assessment through HPC-Integrated Computational Fluid Dynamics
Speaker(s): Maxime Pallud, TotalEnergies |
| 1:30 p.m. – 2:05 p.m. | From Leader to Fast Follower Through the Barren Cloudy HPL Valley
Speaker(s): Gary Grider, Los Alamos National Laboratory (LANL) |

Technical Talks: HPC for Research >> Second Floor, Room 280

- | | |
|--------------------------------|---|
| 12:20 p.m. – 12:55 p.m. | A Tour of Deep Learning Applications for Seismic Processing, Imaging, and Interpretation
Speaker(s): Anatoly Baumstein, ExxonMobil |
| 12:55 p.m. – 1:30 p.m. | GPU Migration for a Seismic Imaging Software Framework at bp
Speaker(s): Muhong Zhou, bp
Author(s): Muhong Zhou, bp; Jonathan Eichelberger, bp; Kent Blancett, bp; Wanying Wang, bp; Elizabeth L'Heureux, bp; Hu Jin, bp; Xukai Shen, bp; Simon Luo, bp; Xiaolei Song, bp; Fatmir Hoxha, NVIDIA; Guillaume Thomas-Collignon, NVIDIA; Guillaume Barnier, NVIDIA; Igor Terentyev, NVIDIA |
| 1:30 p.m. – 2:05 p.m. | Strategic Benchmarking and Acquisition of Next-Generation Supercomputers at ExxonMobil
Speaker(s): Karthik Neerala Suresh, ExxonMobil
Author(s): Karthik Neerala Suresh, ExxonMobil; Kirsten Byers, ExxonMobil; Rahul Sampath, ExxonMobil; Jordan Pomeroy, ExxonMobil |

2025 PROGRAM | WEDNESDAY, FEBRUARY 26

W Add-On Workshop

B Birds of a Feather (BOF)

M Main Session

N Networking

A Technical Talk: Domain Science and AI

R Technical Talk: HPC for Research

S Technical Talk: Innovation and Sustainability

E Technical Talk: Programming and Systems Efficiency

8:00 a.m. – 8:30 a.m.

N Check-in + Breakfast ➤ Auditorium + Exhibit Hall

8:30 a.m. – 9:30 a.m.

B BOF | Texas Women in HPC: Workforce Development and the Rise of AI ➤ Auditorium
Cristina Beldica, Intel Corporation; Kasia Cevallos, Microsoft; Melyssa Fratkin, Texas Advanced Computing Center (TACC); Arianna Martin, bp; Rosalinda Mendez, NOA Research

9:30 a.m. – 10:00 a.m.

N Morning Coffee Break ➤ Exhibit Hall

10:00 a.m. – 10:10 a.m.

M Welcome | Day 2 ➤ Auditorium
Speaker(s): David Pynadath, Ken Kennedy Institute, Rice University

10:10 a.m. – 10:55 a.m.

M Keynote | AI and HPC in the Energy Transition ➤ Auditorium
Speaker(s): Selda Gunsel, Shell Technology

10:55 a.m. – 11:30 a.m.

M Targeting Applications to First-Generation Exascale Systems ➤ Auditorium
Speaker(s): Timothy Williams, Argonne National Laboratory

11:30 a.m. – 12:20 p.m.

N Lunch ➤ Exhibit Hall

12:20 p.m. – 2:00 p.m.

A Technical Talks: Domain Science and AI ➤ Auditorium

12:20 p.m. – 2:00 p.m.

E Technical Talks: Programming and Systems Efficiency ➤ Second Floor, Room 280

2:00 p.m. – 2:40 p.m.

N Afternoon Break ➤ Exhibit Hall

2:40 p.m. – 3:15 p.m.

M Poster Lightning Talks by Graduate Students ➤ Auditorium
Cristel Carolina Brindis Flores, Rice University; Chen Chen, Rice University; Dragana Grbic, Rice University; Max Hawkins, Georgia Institute of Technology; Kashif Liaqat, Rice University; Jason Ludmir, Rice University

3:15 p.m. – 3:50 p.m.

M Fireside Chat with Dan Reed: Thoughts on the Past, Present, and Future of HPC ➤ Auditorium
Speaker(s): Melyssa Fratkin, Texas Advanced Computing Center (TACC); Daniel “Dan” Reed, University of Utah

3:50 p.m.

M Closing Remarks ➤ Auditorium
Speaker(s): David Pynadath, Ken Kennedy Institute, Rice University; Keith Gray, TotalEnergies

3:50 p.m. – 5:15 p.m.

N Poster Presentation Reception ➤ Exhibit Hall

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Technical Talks: Domain Science and AI Auditorium

12:20 p.m. – 12:45 p.m.	Advancing Reservoir Engineering through High-Performance Computing and Neural Operators on the Cloud Speaker(s): Karthik Mukundakrishnan , Stone Ridge Technology; Vidyasagar Ananthan , Amazon Web Services Author(s): Karthik Mukundakrishnan , Stone Ridge Technology; Vidyasagar Ananthan , Amazon Web Services; Dan Kahn , Amazon Web Services; Dmitriy Tishechkin , Amazon Web Services
12:45 p.m. – 1:10 p.m.	MFIX-Exa: Simulations of Chemical Reactors at the Exascale Speaker(s): Roberto Porcu , National Energy Technology Laboratory Author(s): Roberto Porcu , National Energy Technology Laboratory; Jordan Musser , National Energy Technology Laboratory; Ann S. Almgren , Lawrence Berkeley National Laboratory; John B. Bell , Lawrence Berkeley National Laboratory; William Fullmer , National Energy Technology Laboratory; Deepak Rangarajan , National Energy Technology Laboratory
1:10 p.m. – 1:35 p.m.	Reactive Transport Simulation in Porous Media and Implications for CCS Speaker(s): Jeremy First , bp; Yuliana Zapata , bp Author(s): Jeremy First , bp; Yuliana Zapata , bp; Srivatsa Mudumba-Ramana , bp/Numerical Algorithms Group
1:35 p.m. – 2:00 p.m.	Hybrid Quantum/Classical Machine Learning for Molecular Conformation Generation Speaker(s): William Clements , ORCA Computing Author(s): William Clements , ORCA Computing; Hugo Wallner , ORCA Computing; Corneliu Buda , bp; Omar Bacarreza , ORCA Computing; Peter Lemke , bp; Claudia Perry , bp

Technical Talks: Programming and Systems Efficiency Second Floor, Room 280

12:20 p.m. – 12:45 p.m.	A Pragmatic Approach to Optimize Execution Time and Cost of Complex Coupled-Physics Codes in Chevron's HPC Speaker(s): Michael Thomadakis , Chevron Technology Center Author(s): Michael Thomadakis , Chevron Technology Center; Pavel Tomin , Chevron Technology Center; Alex Loddock , Chevron Technology Center; Victor Magri , Lawrence Livermore National Lab
12:45 p.m. – 1:10 p.m.	PGAS-Based Distributed OpenMP (DiOMP) for Seismic Modeling with Extension to GPU Computing Speaker(s): Mauricio Araya-Polo , TotalEnergies EP Research & Technology US Author(s): Baodi Shan , SUNY Stony Brook; Barbara Chapman , SUNY Stony Brook; Mauricio Araya-Polo , TotalEnergies EP Research & Technology US
1:10 p.m. – 1:35 p.m.	Optimizing the Delivery of High-Performance Workstations for Geophysical Workflows in Subsurface Exploration Speaker(s): Stephen Rigler , Chevron Corporation; Blake Ray , Chevron Corporation; Karen Gondoly , Leostream Corporation Author(s): Stephen Rigler , Chevron Corporation; Blake Ray , Chevron Corporation; Karen Gondoly , Leostream Corporation
1:35 p.m. – 2:00 p.m.	Immersed Boundary Abstractions for Constructing Land Seismic Imaging Frameworks Speaker(s): Edward Caunt , Devito Codes Author(s): Edward Caunt , Devito Codes; Rhodri Nelson , Imperial College London; Fabio Luporini , Devito Codes; Mathias Louboutin , Devito Codes; Gerard Gorman , Imperial College London

* If you decide to add-on a Thursday workshop after you have already registered, please reach out to conference staff to update your registration.

FEBRUARY 27 • THURSDAY

8:00 a.m.	W	Best Practices in HPC Systems Management >> 2nd Floor, Room 280
8:30 a.m.	W	Scientific Machine Learning >> Auditorium
8:30 a.m.	W	Devito User and Developer Workshop >> 10th Floor, Room 1003
8:30 a.m.	W	Building an Optimized Elastic Finite-difference Propagator from Scratch for FWI on NVIDIA's Latest GPUs >> Exhibit Hall
8:30 a.m.	W	Performance Evaluation of GPU Accelerated HPC and AI Applications Using HPCToolkit, TAU, and ParaTools Pro for E4S™ >> 1st Floor, Room 106

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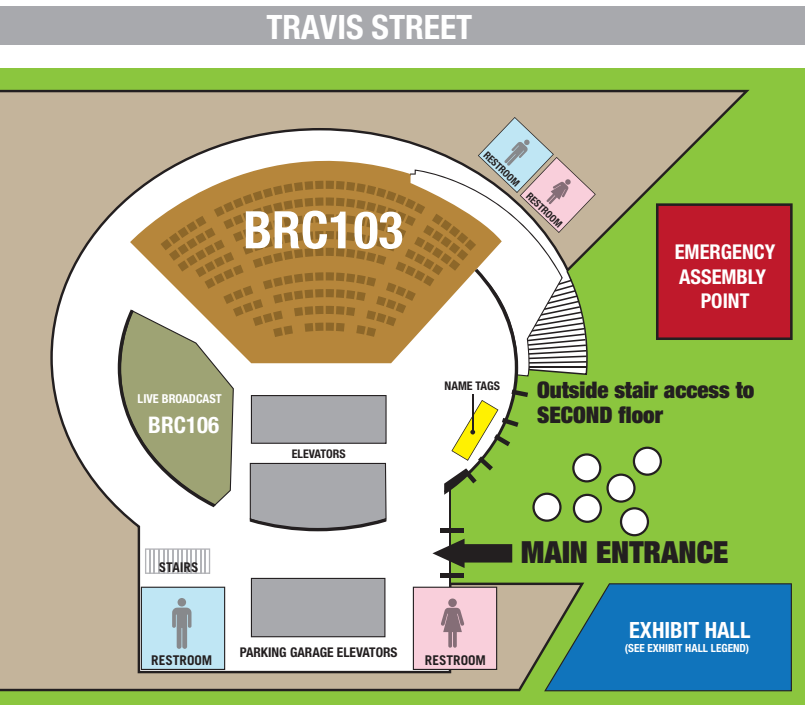
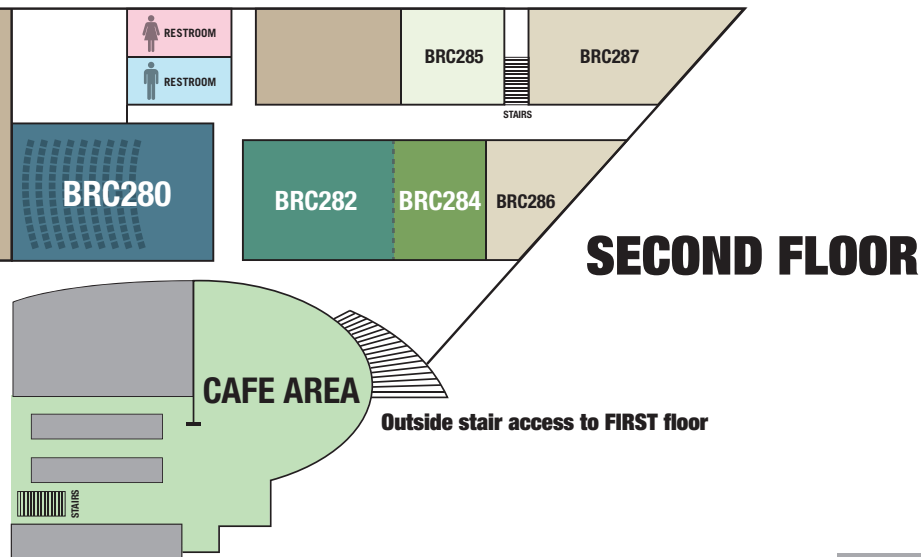
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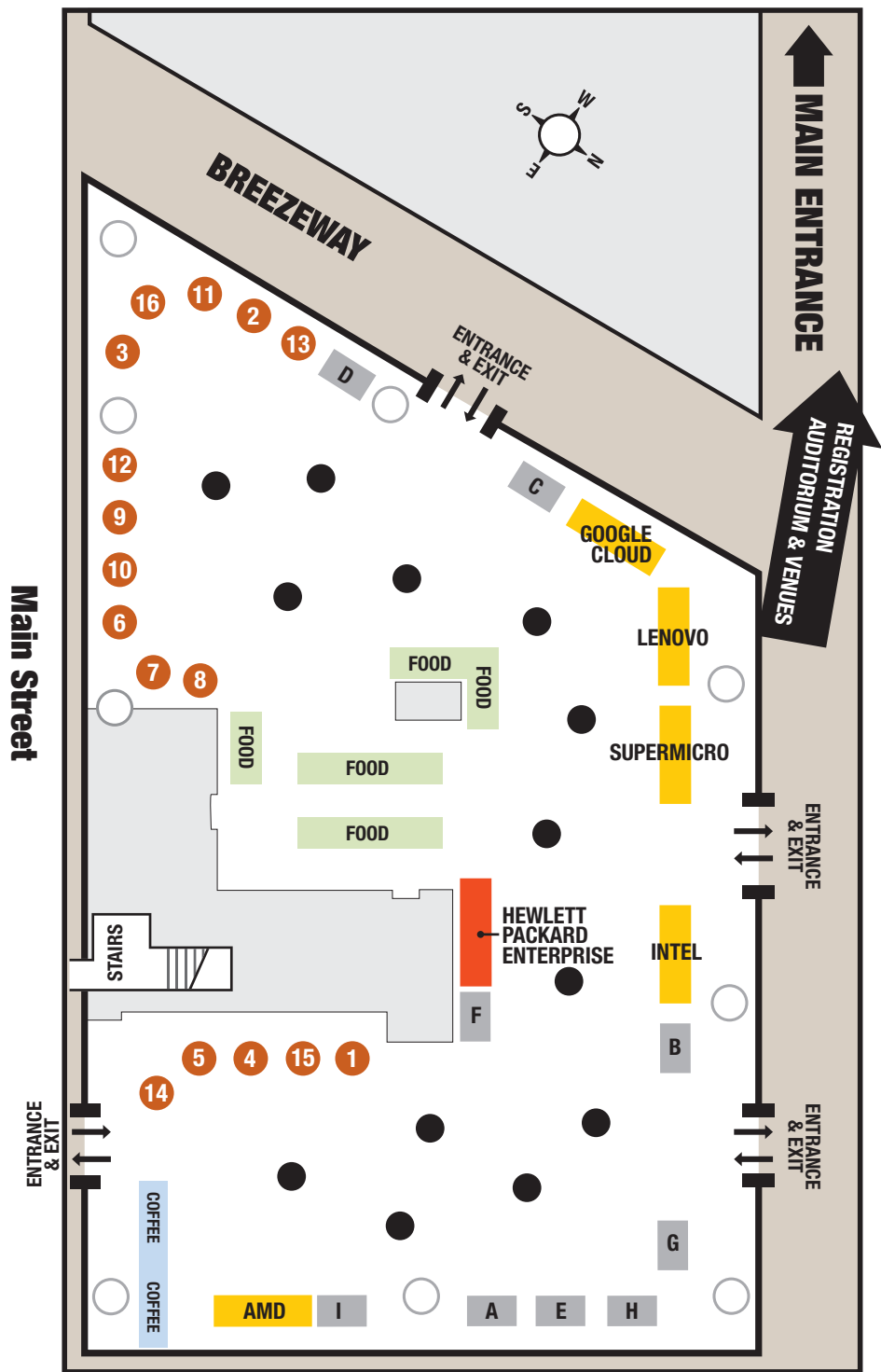
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Texas Women in High Performance Computing

Accelerating Downhole Distributed Acoustic Sensing Data Processing for Borehole Seismic Monitoring

Rosie Zhu (Rice University) and Jonathan Ajo-Franklin (Rice University)

Carbon-Neutral Recovery of Natural Gas from Shale: Sequestering CO₂ While Enhancing Gas Production | Lightning Talk

Cristel Carolina Brindis Flores (Rice University), Walter Chapman (Rice University) and Philip Singer (Rice University)

Confidence and Degeneracy in Parameter Estimation of Biophysical Neuron Models

Anwar Khaddaj (Rice University), Saina Namazifard (Baylor College of Medicine), Matthias Heinkenschloss (Rice University) and Fabrizio Gabbiani (Baylor College of Medicine)

Efficient Monte Carlo Methods for Estimating System-Level Reliability of Power Grids

Ziran Wang (Rice University) and Leonardo Dueñas-Osorio (Rice University)

Energy HPC Orchestrator: A Cloud Native HPC Workflows Management Application

Kun Jiao (AWS), Cyril Lagrange (AWS), Dan Kahn (AWS), Shel Hussein (AWS), Max Liu (Shell) and Marwan Wirianto (Shell)

Enhancing Data Center Energy Efficiency with a Solar Thermal Boosted Waste Heat Recovery System | Lightning Talk

Kashif Liaqat (Rice University) and Laura Schaefer (Rice University)

Integration of Machine Learning, Geospatial Analysis, and Life Cycle Assessment to Determine the Well Pad-Specific Carbon Footprints of Natural Gas Extraction

Amir Sharafi (University of Nevada, Las Vegas) and Marie-Odile Fortier (University of Nevada, Las Vegas)

Learning to Route with Confidence Tokens

Yu Neng Chuang (Rice University), Guanchu Wang (Rice University) and Xia Hu (Rice University)

Leveraging HPC and Advanced Hydrological Modeling for Accurate Flood Forecasting

Girishchandra Yendargaye (C-DAC), Murugesh Prabhu (C-DAC), Upasana Dutta (C-DAC) and Yogesh Kumar Singh (C-DAC)

Measuring and Analyzing Application Performance At Exascale | Lightning Talk

Dragana Grbic (Rice University) and John Mellor-Crummey (Rice University)

One Rank at a Time: Cascading Error Dynamics in Sequential Learning

Mahtab Alizadeh Vandchali (Rice University), Fangshuo Liao (Rice University), Nikhil Chigali (Rice University) and Anastasios Kyriillidis (Rice University)

Optimizing US Industrial Heat and Power Systems with Geothermal Deployment in 2030

| Lightning Talk

Chen Chen (Rice University) and Daniel Cohan (Rice University)

Pluvial Flood Emulation with Hydraulics-Informed Message Passing

Arnold Kazadi (Rice University), James Doss-Gollin (Rice University) and Arlei Silva (Rice University)

Repulsive Latent Score Distillation for Solving Inverse Problems

Nicolas Zilberstein (Rice University)

Reverse Time Migration on the STX Accelerator

Ryuichi Sai (Rice University), John Mellor-Crummey (Rice University), Timo Schlachter (Fraunhofer ITWM), Jens Krüger (Fraunhofer ITWM) and Mauricio Araya-Polo (TotalEnergies EP Research & Technology US)

Runtime and Energy Analysis of SpMV Hardware Execution Choice | Lightning Talk

Max Hawkins (Georgia Institute of Technology), Christian Engman (Georgia Institute of Technology) and Ivan Rocha (Georgia Institute of Technology)

Sensitivity-Driven Surrogate Model Refinement for Trajectory Optimization with Expensive Black-Box Functions

Jonathan Cangelosi (Rice University) and Matthias Heinkenschloss (Rice University)

Sweeping Heterogeneity with Smart MoPs: Mixture of Prompts for LLM Task Adaptation

Anastasios Kyrillidis (Rice University)

The Accessibility and Inaccessibility of Urban Public Charging Station

Hossein Gazmeh (Rice University), Xinwu Qian (Rice University), Mario Small (Columbia University), Qi Wang (Northeastern University) and Yuntao Guo (Tongji University)

Towards Flexible Demultiple with Deep Learning

Mario Ruben Fernandez (Fraunhofer ITWM), Norman Ettrich (Fraunhofer ITWM), Matthias Delescluse (École Normale Supérieure) and Janis Keuper (Offenburg University)

Unbalanced Research Effort: A Comparative Analysis of Energy Research Articles in Commercial and Residential Buildings

Sumeyra Danisman (Stony Brook University) and Elizabeth Hewitt (Stony Brook University)

Unsupervised Quantum Anomaly Detection: Quantum Computing for Detecting Critical Anomalous Events | Lightning Talk

Jason Ludmir (Rice University) and Tirthak Patel (Rice University)



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